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MODERN FOUNDATIONS AND GOALS

G. Gottschalk

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16. Abstract
A definition of modern analytics was given which explained the determination of quality, quantity, and state of components in materials as limited tactical questions within a superposed strategy for an optimal gain and utilization of information on the state and processes in material systems. The basic principles of system theory, theory of games, and information theory were outlined and interpreted from the view of analytics.

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FUTURE ASPECT OF ANALYTICS
MODERN FOUNDATIONS AND GOALS

G. Gottschalk

1. Problem Definition Analytics

Analytical chemistry has understood, and today still understands itself, generally as a relatively narrowly circumscribed science. It provides assertions concerning the kind, amount, and arrangement of certain components in material systems. Tasks put to it are becoming increasingly more complicated, with respect to the number of relative components, and with respect to the interrelationship and effect of these components. This make the personal labor and the expense of equipment required for the tasks more and more specialized, more expensive, and often more time consuming. As long as chemical analysis regards itself as a link in the chain of order/analysis/use, it will not succeed in escaping the widely spread view that it is indeed quite a necessary, but, in the long run, only a service-providing auxiliary science. The analyst remains a more or less esteemed "speciality idiot," or he remains trapped in a narrow professional area of effectiveness, as an arbitrarily replaceable "service organ." A relatively small chance for advancement to higher management positions, and an early attainment of a not very lucrative salary limit are adequate reasons for future academic generations to avoid this profession, or to leave it as quickly as possible, as these realizations grow. This unhappy professional picture predominates primarily in the Federal Republic of Germany, where the few chairs for analytical chemistry are rarely adequately endowed in terms of working force and finances. /1*

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*Numbers in the right-hand margin indicate pagination in the foreign text.

Here arises the question of whether the analyists with their conception of analytical thinking and acting are completely guiltless in this situation. A few considerations relative to the future are offered below. The goal of analytical activities is, even today, still seen mainly in terms of the following questions:

What is there? (Qualitative Analysis)
How much is there? (Quantitative Analysis)
How is it disposed? (Structural Analysis)

These quite clear and comprehensive interpretations of the area of /2
analytical work cast the shadow of illusion over the fact that such analytical activity is only a tactical step within the framework of defining over-riding problems. Definitions of over-riding problems are, for example, the optimizing of material properties and production processes, questions of quality, or the numerous future tasks of protection and control of the environment. The solution of such over-riding problems requires a strategic conception. A strategic conception regards an analytic problem not as a limited task of pure material object analysis, but seeks to include the causes of the task and the effects of the results in its overall considerations. The more or less isolated performance function of the analyst must here be enlarged by significant planning and consulting functions. The too narrowly limited concept, "analytic chemistry" should be supplanted by the more comprehensive concept "analysis," and "material" should be replaced by "system" and "analyst" should be replaced by "system analyst." The "system analysts" enjoy growing esteem in the age of automation and information science; they appear as a kind of magician, who can disentangle opaque and enmeshed connections, regardless of kind, with new methods of thinking.

What else does the analytical chemist do? The experience of the author has, at any rate, shown that the step from the purely chemically oriented analyst to the universal system analyst is easier than in most other professions. This is in no way surprising, since a good chemical-analytic education transmits at least implicitly all the knowledge and postulates that are essential for system-analytic thinking and acting.

Let us therefore ban the too narrow "what, how much, how" from the professional image of the analyst, and let us define anew, as a requirement and a duty of the future:

> Analysis provides optimal strategics for obtaining and utilizing relevant information concerning conditions and processes in material systems.
>
> Chemically oriented procedures and methods are here tactical aids for attainment of partial goals.

The enlarged analytical thinking and acting first of all requires additional knowledge from the areas of cybernetics and information theory which has hitherto scarcely been considered in the education of the chemist in the Federal Republic of Germany. At the technical college in Vienna, by contrast, remarkable programs have been developed. to include system and information theory in the curricula of the chemist. Several new scientific areas and their connection with analysis will be briefly sketched from the new viewpoint in what follows.

2. System Theory

System theory can be regarded as the basis for all modern methods of thinking. This is reason enough for the work group "Automation in Analysis[1]" to have occupied itself with this area extensively last year. In a first publication on the topic "System Theory in Analysis" [11] twelve basic concepts of system theory concepts were defined in general and were specially interpreted from an analytical point of view. These concepts are: system,

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[1] In April 1966, at the Analysts Convention in Lindau, a work group was founded, comprised of professional colleagues from Germany, Austria and Switzerland.

element, relation, function, structure, organization, feedback, black box, model, input-output analysis, trial-and-error method, and simulation. Beyond this, a system oriented work technology is described for analysis or for the creation of new systems, where the feedback work steps of qualification and modification of problem definition/limitation/model creation/simulation are illucidated under the mnemonic PAMS. Figure 1 shows a further general scheme of the system-oriented process.

With a view to the consistent planning and documentation of analytical processes and methods, a consistent definition and interpretation of system theoretic elements and of relations in the special system of analytical quantification are necessary. The concept such as "macro, ultramicro, submicro, etc." today find more or less arbitrary use in various connections and orders of magnitude, and are inconsistently interpreted. The system analytic decoding of this special problem area in analysis resulted in the necessity of differentiating three subsystems:

Work areas (quantification of the comprehensibility of a given component X). /3

Sample quantity (quantification of a sample substance component X plus matrix Y, X + Y).

Content (quantification of the relation $\frac{X}{X+Y}$).

This problem definition currently is being worked on by the above-named work group in close contact with many professional colleagues. Uniform agreement in terminology is a necessary precondition before analytical-chemical information banks can be set up. The activity sketched is an essential tactical step in a future-oriented strategy, whose goal is rapid access to analytical information. Care must here be taken that analytical information be intelligible, at least in certain parts, not only to chemists, but also to biologists, physicians, engineers, businessmen, and even to lawyers and politicians. The making of legal decisions and of laws, concerning transgressions and prescriptions in the area of environmental protection, for example, requires additional interpretation by the specialist for matters of analytical-chemical fact. This must be especially emphasized. But a common system analytic manner of thinking of chemist, lawyer, and politician, can contribute decisively to rapid understanding and to the avoidance of misunderstandings.

3. Game Theory

Von Neumann and Morganstern, in the years 1928-1943, developed the principals of modern game theory. These were published in "Theory of Games and Economic Behavior." A short and comprehensible introduction to the mathematical foundation is given by Vogelsang [12]. The most important concepts of game theory are collated and defined in Figure 2.

To prevent misunderstanding the ambiguous German word "Spiel," it should be pointed out that the English word "game" is understood more in a sense of "competition" than in the sense of "enjoyment" (play). It seems comprehensible that game theory resulted first of all in insights concerning the

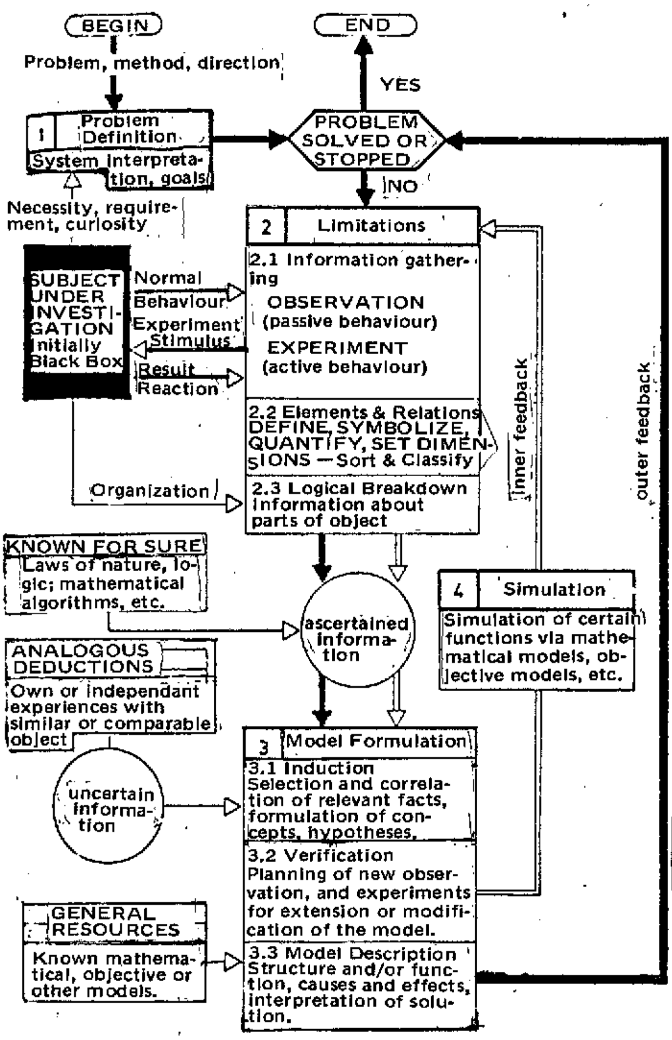


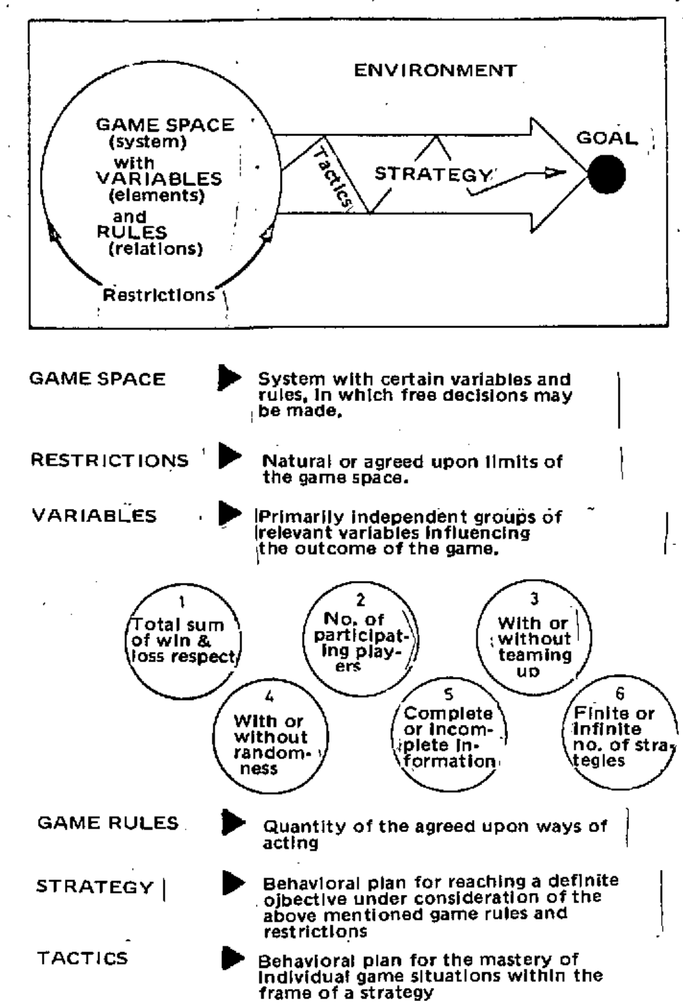
Figure 1. System oriented approach.

optimal formation of economic planning processes, since the competition character is particularly sharp in the game area of the "market." Many methods of operations research were developed from game theory investigations, and were taught in the form of "enterprise games." The behavior of management by objectives and of management by exceptions can also be interpreted by game-theory variants of a strategic or tactical orientation in thinking and acting. Game theory can be regarded as a special case of general system theory. In the special system game space, the relations permitted by the rules of the game are realized on the basis of free decisions in a more or less random sequence, where running through the possibilities generally corresponds to a simulation.

The analyst too acts within a game space, which includes laboratories, personnel, and aids such as equipment, apparatus, and automatic machinery. He obtains or chooses certain objective goals in his work. Generally, he clearly recognizes the objective restrictions in the form of the state of knowledge in chemical analysis, personnel qualifications, and equipment. But the younger /4
colleague in particular is not clearly aware of the restrictions of a planned economy in the form of three characteristic complexes: work capacity, time, and cost. At any rate, they are regarded as a bothersome constraint on his activities. The three named restricted characteristics are collated and explained in Figure 3.

These named restrictions demand that a conscious evaluation be made of the actual situation and the situation of interest, in the acceptance and execution of analytic tasks, and in the formulation of investment wishes with respect to new devices for analysis. Their inclusion in a planning process will be shown in an example of an analytic research group, details of which cannot be discussed at this point.

Here we have only a sketched outline of the economical aspects on analytical factual questions. It is evident that this places the analyst in a position to quantify the value of his work and



Basic Variables:

Planning interval:	1 calendar year = 1 working year
Average no. of personnel:	N = 10 people
Approved budget:	B = 400,000 DM
Service demanded:	L = 40,000 DM
Total cost:	K = B + L = 440,000 DM
Calc. basic values:	KJ = K/N = 44,000 DM/man yearly
	KD = KJ/220 = 200 DM/man daily
	KH = KJ/1760 = 25 DM/man hourly

Variables for a certain analytical problem definition

Work capacity required:	probably x = 30 Md (max. 40, min. 24)
Personnel available:	probably y = 2 (max. 3, min. 1)
Dates:	Probably $z = x/y$ = 30/2 = 15 Ad
	Max. z = 40/1 = 40 Ad
	Min. z = 25/3 = 8 Ad
	Set calendar dates for beginning and ending days
Labor costs:	probably a = KD x x = 6000 DM
	Max. a = 200 x 40 = 8000 DM
	Min. a = 200 x 24 = 4800 DM

Variables for investment justification

Time span:	1 year
Work capacity required: till now:	x_1 = 300 Md
with new equipment:	x_2 = 100 Md
difference:	Δx = 200 Md
Cost effectiveness: direct:	n_1 = KD x x = 40,000 DM
indirect[2]:	n_2 = 60,000 DM
total:	n = 100,000 DM
Investment: absolute:	u = 200,000 DM
amortization time:	$t = u/n$ = 2 years

Figure 2. Concepts of game theory. Game theory aids in the selection of optimal behavior in decision situations.

to prove that he furnishes first-rate information at marketable prices. At present, analytical education scarcely reaches modes of thought and behavior, let alone embodies them in a training program. It would be desirable for consideration to be given to this point in the future.

In this connection it must be asked why there are still no

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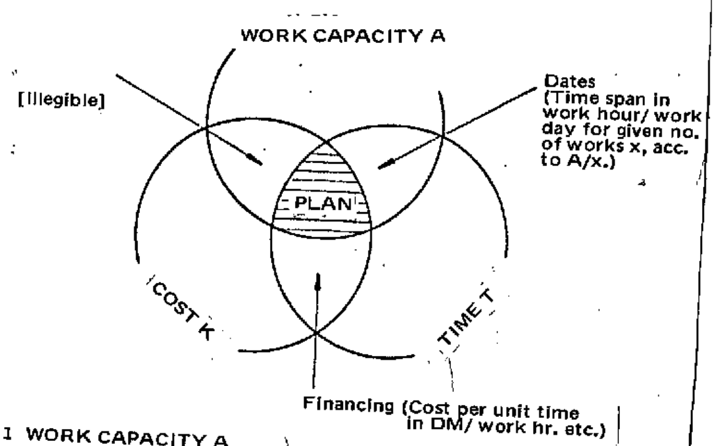
[2]For example, estimated recognized value or value of the savings in energy, waste, etc., by means of faster execution of analysis and others.

analytically-oriented management games. Purposeful games can effectively promote the learning and application, especially from relations. /5



1 WORK CAPACITY A

Basic Parameters: WORKERS - TIME (manpower)
Units: Manhour to man year (Mh, Mj)
Presently used: *1 man day Md = 8 Mh*
1 man week Mw = 5 Md = 40 Mh
1 man month Mm = 4 Mw = 20 Md = 160 Mh
1 Mj = 11 Mm = 44 Mw = 220 Md = 1760 Mh

2 COST K

Basic Parameters: Means of Payment
Units: e.g. DM and TDM = 1000 DM
Costs are global variables, consisting of personnel and material costs K = Pk + Sk. Quantities used in cost calculations are e.g. budget B and Service L (negative costs). K = B + L and B = K - L respectively.

3 TIME T

Basic Parameters: PRODUCTION TIME and DATES

Units: Work hr Ah (Calendar dates)
to work year Aj (Calendar days)
(Date)

Presently 1 Ad = 8 Ah. Number of possible Ah differs from calendar year to calendar year, which juxtaposes calendar days and work days. If multi-shifts are used, one calendar day may contain as many as 3 Ad.

Figure 3. Restriction characteristics.

Weisz [13] has shown that "analytical games" are not unrealistic. He developed a chemical-analytical game with 32 cards and 4 players which permits vast number of chemical reactions to be played through. The cards denote 19 metals and 12 reagents. Players 1 and 3 and players 2 and 4 form teams. An example of a round is:

1 plays Hg card

2 trumps with HCl card (precipitation!)

3 trumps with H_2S card (conversion to sulfide)

4 discards a metal or reagent card with low point value.

The round goes to team 1 3. This game enjoys great popularity with students and assistants although one must also occasionally consult a text for clarification of the state of affairs or must conduct an experiment. Huizinga [5] speaks of the "Homo ludens" and proves, that the instinct of play in man has contributed decisively to cultural achievements.

4. Information Theory

Information theory is concerned with the principles and possibilities of transmitting and processing information. On the other hand, the aim of analytics is the production and utilization of relevant information on material states and processes. In this regard the actual analytical investigation and documentation includes transmission and processing of information. Hence, the perceptions of information will in the future be of essential significance, for optimum design as well as for evaluation of the efficiency of analytical methods and devices.

An information system is a special system in the sense of the system theory. Its relevant elements are characterized by the concepts S i g n a l and S i g n and its simplest relations by relations = C o d e between different signal or character sets. The potential appearing at a glass electrode is in the first instance only a signal. The signal value in the millivolt range is decoded by means of a rather costly, related apparatus "pH-meter" for indicating pH. Ultimately, every analytic function is a Code because it describes the relation of signals = measured values to sign = analytical quantities. The interaction between two or more information systems, for example, between an analytical device and an analyst (machine/man) or an interested party/analyst (man/man), means communication. For this reason information systems are subsystems of a higher ordered communication system. In this context the concept, communication, is used in a summary fashion for the special relations between subsystems.

Input and output information lead by way of the information systems to the concepts transmitter and receiver. A channel for transmission of information in the form of signals must be placed between the two. The pure transmission of information is characterized by coding and decoding processes. Here one must distinguish between spanning space = transmission and spanning time = storage. The actual processing of information is, however, a far more complex process which runs through many levels. These levels are characterized /6 by the concepts of syntactics, sigmatics, semantics, and pragmatics and collectively by semiotics.

On the syntactical level only certain rules for a permissible combination are given. They are combinations of prescribed or freely chosen signals or equivalent signs for certain sequences or patterns. There evolves a sort of artificial or "synthetic language" with "synthetic words and sentences." On the other hand, natural and artificial languages allow syntactical elucidation. The syntactical relations are called syntax and, in the case of natural languages, this is also designated as grammar. Computer languages, such as Algol, Fortran or Cobol, are typical examples of artificial languages with relatively simple, yet quite singularly defined, syntax. They were developed for the purpose of man/computer communication. The chemical language of symbols is also an artificial language. Here the series of signs, as for chemical combination laws and reaction equations, or sign patterns, such as structual formulae and spatially structured figures, are constructed along usually uniform rules. As a consequence, part of the "chemical syntax" was internationally adopted into the "Guiding Principles for Nomenclature of Inorganic Compounds" of the IUPAC[3] [9]. Syntactical problems can be handled with mathematical-statistical methods. Concepts such as I n f o r m a t i o n C o n t e n t, R e d u n d a n c y and others are syntactical state variables. They are based on processes for selecting signals and signs from certain previously defined supplies. Each required decision in the frame of selection is thereby counted with the unit 1 bit. Figure 4 gives a summarized survey of the essential syntactical parameters, particularly as Shannon [10] has formulated it.

It was Kaiser [6], as well as Doerffel and Hildebrand [3], who set forth the first formulations for interpreting the "Information Contents" of analytical methods and apparatus on the /7 basis of Shannon's formula, in order to obtain comparable ratings. But even today it is already being said that a satisfactory solution to these problems is not possible on the syntactical level alone, because a pure bit-count still allows no problem oriented valuation of the respective analytical information system. This too Kaiser has already pointed out. Why this should be so is briefly outlined in an example:

The sign sequence, arranged in words and sentences,

all Eilaka'n are Esab'n. Muidibur is an Eilakla, so it is an Esab	or	All Wudeln are Schnurden. This Gagboe is a Wudel, so it is a Schnurde [2].

,

[3]IUPAC = International Union of Pure and Applied Chemists.

INFORMATION CONTENTS $I = -\mathrm{ld}\, P_i$ bit

with $0 < P_i < 1$ and $\sum_i^n P_i = 1$

defines the number of binary decisions for the representation or selection of an event *i* (signal, sign, characteristic, etc.) from a set of *n* different events. P_i is the probability that event *i* will occur. If the occurrence is equally probable, we obtain $I = \mathrm{ld}\, n$ bit, because of $P_1 = P_2 = \ldots P_i = P_n = 1/n$.

To represent the n=1- equally probably decimal numbers 0—9, one theoretically needs $I = \mathrm{ld}\ 10 = 3.322$ bit, which in reality turns out to be 4 bit, since 1 bit is the smallest unit (ld = log to base 2 = logarithmus dualis).

AVERAGE INFORMATION CONTENTS $H = -\sum_i^n P_i \cdot \mathrm{ld}\, P_i$ bit event

(Shannon-formula)

For the special case of equally probable events: $H = \mathrm{ld}\, n = I$ bit/event

n = I bit/Ereignis

REDUNDANCY absolute $R = H_{max} - H$ bit/event

relative $r = R/H_{max}$

defines the required or empty "surplus information"

For the equally probable decimal numbers $H = 3.322$ bit/digit bit/digit.

Practically, one needs $H_{max} = 4$ bit/digit; therefore, the redundancy $R = 0.678$ and $r = 0.1695$ or 16.95%, respectively.

INFORMATION QUANTITY $I_m = z \cdot H$ bit

defines a sequence or sample of z events.

INFORMATION FLOW $I_f = I_m / t$ $\mathrm{bit} \cdot \mathrm{s}^{-1}$

defines input or putput of information per unit time.

INFORMATION DENSITY $I_d = I_m / F$ $\mathrm{bit} \cdot \mathrm{cm}^{-2}$

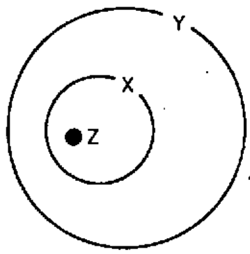
defines a density per area (punch card, tape, disc, etc.)

$I_d = I_m / V$ $\mathrm{bit} \cdot \mathrm{cm}^{-3}$

defines the lesser used density per volume (human brain)

Figure 4. Basic quantities of information theory.

is just as correct according to the syntax of everyday language as it is according to the mathematical-logical syntax, for with E i l a k l a = X, E s a b = Y and M u i d i b u r = Z the logical conclusion is valid:



$$\begin{array}{l} X \subset Y \\ \underline{Z \subset X} \\ \text{so } Z \subset Y \end{array}$$

This applies equally as well for W u d e l, S c h n u r d e and G a b o g e. One recognizes that the information, which is formalized only on the syntactical level, must not necessarily be "generally understandable" and therewith also "utilizable."

On the sigmatic level, concrete or even mental objects or processes are associated with a certain sequence or a pattern of signs so that a plant of certain height and form receives the designation "Baum" (tree).

The sign sequence "Natrium" (sodium) was assigned to a silvery metal with certain physical and chemical properties. One finds a special aspect of the rationality in the sigmatics of the chemical symbols which are independent of the colloquial language. W signifies "Wolfram" as well as tungsten. Another form of rational sigmatics is the application of iconic symbols which convey a pictoral, stylized representation of the designated object. Such icons are found on traffic signs as well as defined picture symbols in electrical diagrams and chemical processes. The advantage of iconic representation of processes lies in the information concentration of facts and in exposing the most essential relations in pictorally abbreviated form. Only in this way does it become at all possible to have a faster overview, a more critical comparison and a direct evaluation of the different kinds of procedural modes. Thus one can, in a significantly shorter period and with much more intensivity, be informed about a complex problem range. So far, a general agreement is lacking on iconic symbols as particularized for the description of analytical processes. Nevertheless, preliminary suggestions, in this regard, are under consideration by Malissa and Jellinek [8]. An additional problem for the future is the creation of an efficient and analytically oriented system of iconic picture elements in order to utilize analytical information in a faster, better and more directed way. Figure 5 shows a compilation of methods used in five laboratories for detecting molybdenum in tungsten materials. It applies the established Malissa/Jellinek symbolism used in the execution of ring experiments.

Even now, in the field of sigmatics, as in syntactics, general intelligibility is by no means a prerequisite. In syntactics, words and sentences are synthesized or analyzed according to statistical rules; in sigmatics, certain objects and processes are only represented by certain words or sentences.

On the semantic level a meaning is assigned to the natural or synthetic words and sentences. Concepts ensue out of "empty" words and their "characterization" of objects and processes. The related "conceptual contents" = meaning must be defined, interpreted, learned and stored. The knowledge, so stored, qualifies the intelligibility of a message. Often there exist simple ciphers by which an unintelligible message can be made into an intelligible one. With the cipher "Read Backwards" there comes from the unintelligible word E i l a k l a'n the concept alkalien, from E s a b'n comes basen and from M u i d i b u r comes rubidium. By comparison there must first be a meaning constructed for W u d e l, S c h n u r d e and G a b o g e. The meaning of natural or synthetic words and sentences is like the main portion of an iceberg which lies beneath the surface. Only the concepts

are directly visible as tips. The difficulty of communication, especially with man as the sender and the receiver of information, is essentially that they very often impute different conceptual contents to the concepts known to them. Table salt has only the meaning of seasoning for the housewife, for the chemist it is a synonym for sodium chloride, a compound of the chemical elements /9
sodium and chloride, something that dissolves in water by dissociation, and, and, and... In contrast to syntactics, it has not yet been possible to satisfactorily embrace semantic aspects mathematically. Because of this the construction of "intelligent machines" is, for the present, placed within narrow limits. Interesting formulations and reflections on the semantic problem are derived by Bar-Hillel and Carnap (Description and Literature See [2]).

In conclusion the value of information is investigated on the pragmatic level in relation to one or more receivers. At present there are no general criteria for the judgment on the information value, still this judgment should be differentiated between an objective and subjective value. One can also speak of a pragmatism of interest. The objective value stands in close connection with the object related completeness and precision of the information itself. A statement of content--"H=64 percent by weight of copper,"--doubtless possesses a lesser objective value than, for example, the statement--"H=62.13 $\pm$ 0.25 percent by weight of copper (n=4, S=99%." In the latter case the range of confidence of the average value, the number n of the number of determinations performed and the statistical certainty S are also specified. The instruction--"dissolve in acid"--is also objectively of less value than the more precise instruction--"dissolve in 10.0 ml 5 M HNO_3." The pragmatic aspect of the objective value also comes to bear on the verbal description--"silver ions react with chlorine ions and precipitate silver chloride"--and the apparent equivalent formulation--"$Ag^+ + Cl^- \rightleftharpoons AgCl\downarrow$." Although the verbal information contains a considerably greater quality of statistical

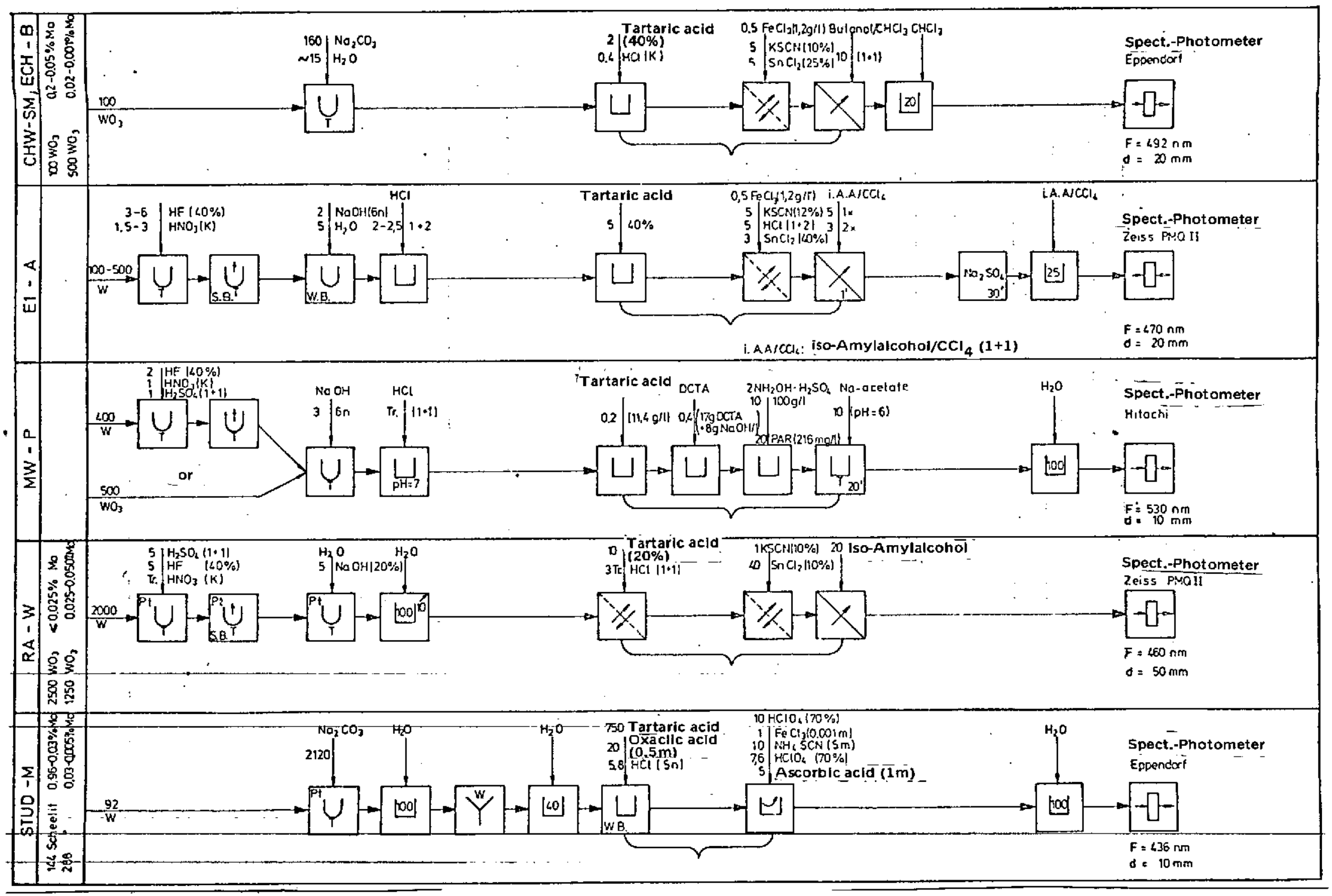


Figure 5. Comparison of analytical methods for the determination of molybdenum in tungsten, as of 2/71-3/71, the beginning of the ring investigation.

information than the reaction equation, it possesses a much smaller objective value. The chemical formula, even with fewer bits, informs more completely and precisely because it also provides the ionic charges, equation of combination as well as molar quantity and equivalence before and after the completed reaction. By contrast the verbal information also permits the interpretation-- "$2\ Ag^+ + Cl^- \rightleftharpoons Ag_2Cl^+\downarrow$" or "$Ag^+ + 2\ Cl^- \rightleftharpoons AgCl_2^-\downarrow$". In this case, however, it is even objectively "false" according to chemical semantics since, as a consequence of colloidal formation, a precipitation does not occur at all. The objective value is measured in adherence to syntactic and sigmatic formalisms, especially with machines and automatons as receivers, in which the semantic background is missing or, for the moment, trifling.

A formal error, in a computer program for example, can make the respective information no longer processable, that is, objectively worthless. The subjective value states whether the existing receiver is interested objectively or temporally in the concerned information (man) or if the receiver can process the information directly (machine). Therefore an objectively high purity value possesses a subjective value only for such human receivers, which want to judge, or must judge, the quality of a product (real value). If, however, he receives the information too late, then its subjective value can be considerably reduced (time value). The subject value information, in the form of a series or of a pattern of signals, and having machines or automatons as receivers, is dependent upon whether the signal events are, on the whole, completely recorded by the associated receivers. If the signal events partially exceed the allowed technical limits of the receiving agents then the subjective value of this information is inferior. A computer program in A l g o l is subjectively worthless, if the computer system in question possesses no A l g o l -compiler as a receiving agent. The objectively valuable signal of the potential at the glass electrode was subjectively of little value as long as no reliable high ohm circuits existed.

It will not be possible to have an optimal analysis in the future without the inclusion of information theory. Specifications of precise basic concepts and their analytical interpretation is an extraordinarily difficult but absolutely necessary task. The reflections outlined here, as well as the works of Kaiser [6] and Malissa [7, 8] are only a beginning.

5. Analytics and Automation

The work group "Automation in Analysis" defines the concept "automaton" as a "construction with mechamisms and instrumentattions which is a closed information system" [1]. This definition requires the existence of an internal i n f o r m a t i o n p r o c e s s e r, independent of man, as essential to the concept of automatons. Accordingly, a titrimetric automatic applies only if the associated construction yields a complete titration result in the form of data relative to the end point. An independent execution of the titration process and the printing or plotting /10 indications of the individual titration data implies only a mechanization and instrumentation. This does not mean that the associated construction does not contain, for example, an automatic dosimeter which regulates the amount of titrant added on command from the respective potentiometric change of a specific electrode. Here, however, only the dosage is automated, not the entire titration process. One speaks of mechanization if a man-operated physical function is augmented or completely taken over by a mechanism or a machine. So, for example, the mixing of a solution by manual rotation or stirring with a stirring rod can be taken over by a motor driven agitator.

Besides the relief of the physical burden, the mechanization, in most cases, also permits more precise information about the process in question. Hence the statement,--"magnetic stirrer with stirring rod of 4 cm ∅, stir 10 minutes at 50 revolutions per minute"--possesses pragmatically a greater objective information value than the statement=="shake well." Instrumentation extends the possibilities of extracting information. An appropriate instrument converts analytically informative signals, which the human senses can grasp only qualitatively if at all, into perceptible signals such as meter readings, number sequences, etc. If the reader is a non-human device, then the signal conversion is limited to the generation of directly utilizable signals, such as analog/digital converters. The temperature, which is perceivable only subjectively and qualitatively as "cold, warm or hot," becomes objectively and quantitatively comprehensible as measured values by means of the instrument--thermometer or pyrometer. The signal transformation through instrumentation must not be equated to a processing of information. As much as ever, the machines and instruments must first be operated by man. Through him, definite relevant information must first be evaluated and converted into a sequence of events. Even with "switching intervals" of 1 to 10 milliseconds, interrupted by "recovery times" of the same magnitude which are physiologically necessary, man's reaction capability is, from the outset, individually different and very limited. The instrumentation for information acquisition IIG[4] is becoming increasingly faster. Pitted against this is a human information processor MIV[5], which is strongly vacilating and, in addition, very slow. The MIV can always be replaced by an automatic information processor AIV[6] which is frequently a million fold faster and, in addition, more reliable. It is only required that the individual steps of the process are foreseeable, invariable as well as programmable in algorithm form and criteria, and structurally manageable. Figure 6 should make clear the effect of the automation

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[4] IIG = Instrument Information Production.

[5] MIV = Human Information Processing.

[6] AIV = Automatic Information Processing.

upon the work sectors: planning/execution/evaluation.

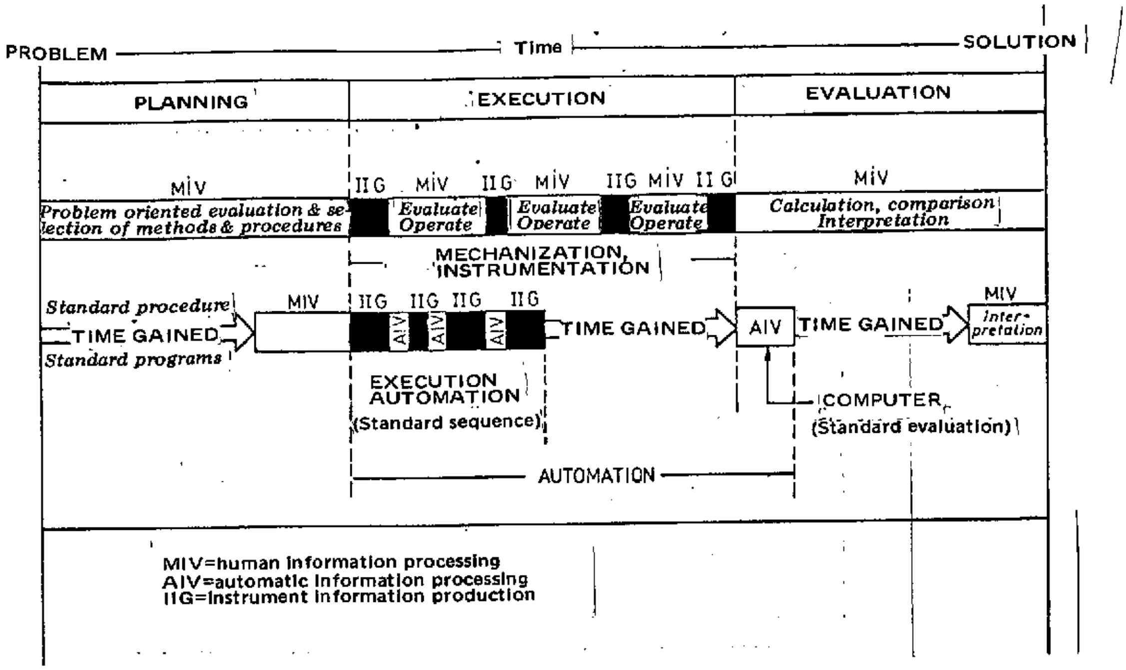

Figure 6. Type and effect of automation in the analysis.

One must not overlook, however, that despite higher working speed and reliability, the automatons work primarily on the relatively primative syntactic and sigmatic level according to rigid, preset rules of the game. In particular, the acceptance of automatons as black boxes contains the risk of "high speed production of nonsense with highest reliability." For the most favorable introduction of automatons into analytics with minimal risks, one must apply a semantically thought out and well directed standardization of the analytical process, sequence of operations and evaluation. In the sense of a step-by-step systems analysis, the formulation of the problem of the standardization of processes lies in the formation of an information system which is applicable to certain types of analytic processes such as titration, /11 photometry, atomic absorption, mass spectroscopy, etc. The processes should also be uniformly and universally applicable to the investigation of any object and to different types of technical fields. Additionally, in the future, valuation criteria must be included at the outset in the educational field of the chemical profession. Research and applications stemming therefrom must be exercised in case studies.

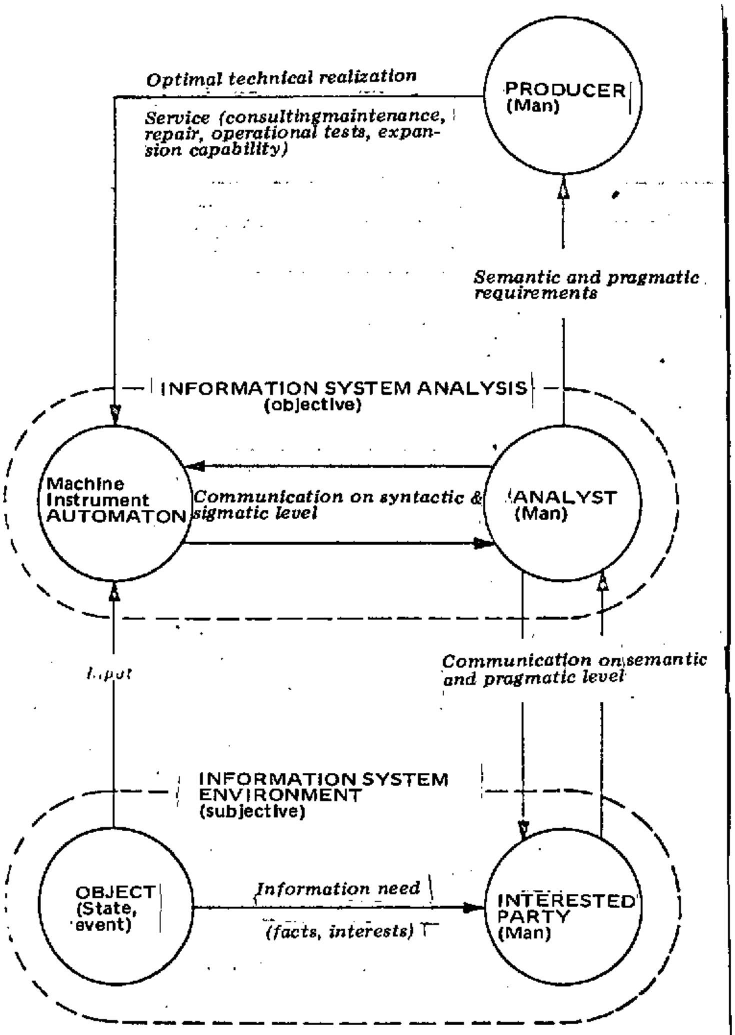

Figure 7. Man and machine in the analysis.

Valuation criteria such as range of quantities, error magnitudes, selectivity properties, limits of detection, degree of difficulties, time requirements, expense of equipment and cost are essential parameters of analytical processes. The standardization of operational procedures follows from the definition and interpretation of individual analytical steps in a process relating to a type of building block system. As a consequence of this, the expanded Malissa-Jellinek symbolism and a chemically oriented network technique represents essentially methodical fundamentals. Test and control methods also belong to the standardization of the ongoing process. These methods yield relevant statements on the limits of the efficiency and the satisfactory functional performance of instruments and above all of automatons. Frequent and serious /12
deficiencies exist in this respect, particularly with analytic automatons, and the analyst is often dependent on slanted psychological advertising and insufficient operational testing by the manufacturer. The standardization of evaluation strives toward the establishment of universally applicable programs which make possible a uniformity of the calculation process as well as a rapid comparison and extensive objective valuation of the results. A general survey and suggestions for the solution of the above problems are found in [4].

In conclusion, Figure 7 shows the relation between man, objects and automatons in diagrammatic form.

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